

Ergostanol

(24«alpha»-methyl-5«alpha»-cholestan-3«beta»-ol)

TMS

InchiKey:

InChI=1S/C31H58OSi/c1-21(2)22(3)10-11-23(4)27-14-15-28-26-13-12-24-20-25(32-33(7

NJILTSJLEGHFOM-YORBPZOMSA-N

Formula:

C31H58OSi

SMILES:

CC(C)C(C)CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C

Mol. weight [g/mol]:

474.88

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.21		Crippen Method
logp	9.574		Crippen Method
rinpol	3216.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R435779&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws:

Log10 of Water solubility in mol/l

logp:

Octanol/Water partition coefficient

rinpol:

Non-polar retention indices

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<https://www.cheméo.com/cid/61-543-1/Ergostanol-24-alpha-methyl-5-alpha-cholestan-3-beta-ol-TMS.pdf>

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